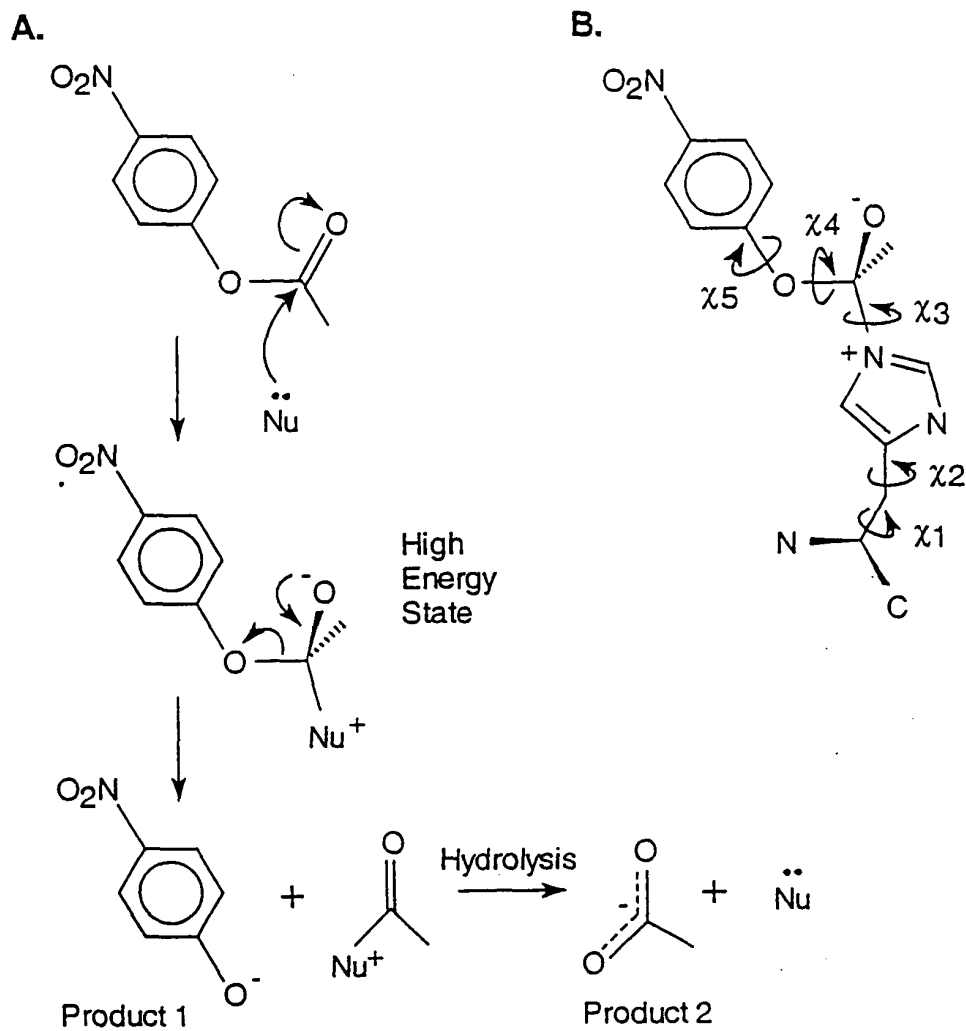Figure 1

PROVIDE SCAFFOLD PROTEIN BACKBONE STRUCTURE

ESTABLISH POSITION IN BACKBONE FOR HIGH ENERGY STATE ROTAMERS

ANALYZE INTERACTION OF HIGH ENERGY STATE ROTATMERS WITH PROTEIN SCAFFOLD TO GENERATE PRIMARY LIBRARY OF VARIANT SEQUENCES WITH PUTATIVE ENZYME-LIKE ACTIVITY

Figure 2

A.

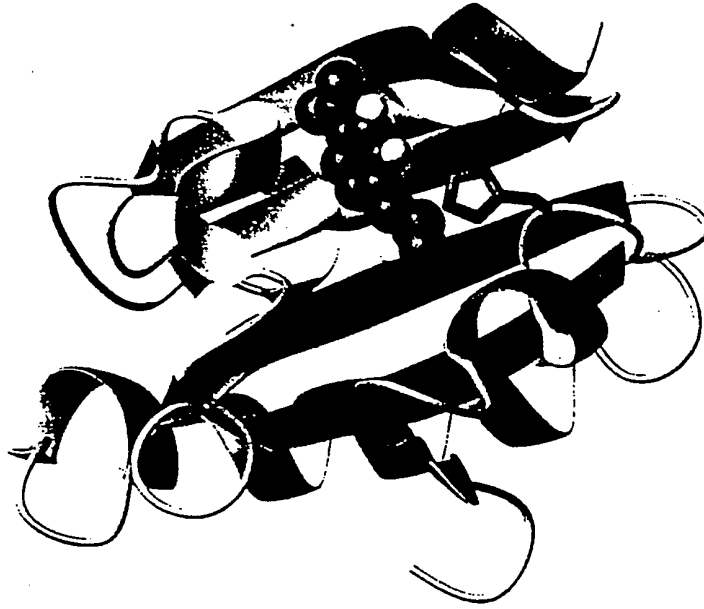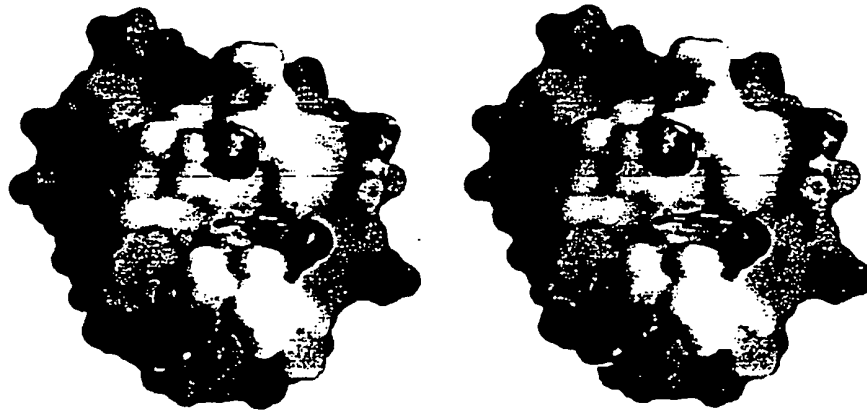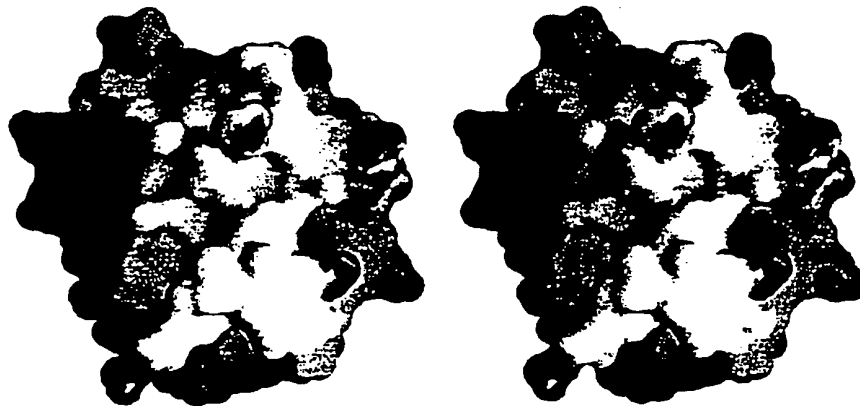High Energy State

Product 1 + Nu⁺ — Hydrolysis → Product 2 + Nu

B.

Figure
3

Figure
4

A.

B.

C.

Figure
5

$$E + S \underset{}{\overset{K_s}{\rightleftharpoons}} E \bullet S \overset{k_2}{\longrightarrow} EI \overset{k_3}{\longrightarrow} E + P2$$

$$\downarrow$$

$$P1$$
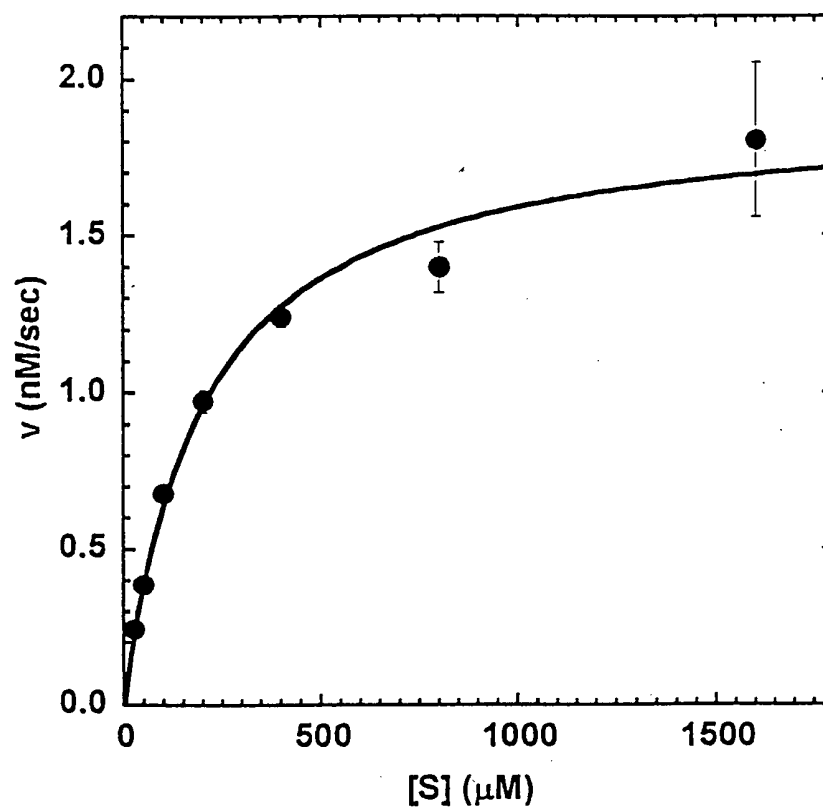
$$v = \frac{k_{cat}[E][S]}{K_m + [S]}$$

$$k_{cat} = \frac{k_2 k_3}{k_2 + k_3}$$

$$K_m = \frac{K_s k_3}{k_2 + k_3}$$

Figure
6

Figure

7

Figure
8

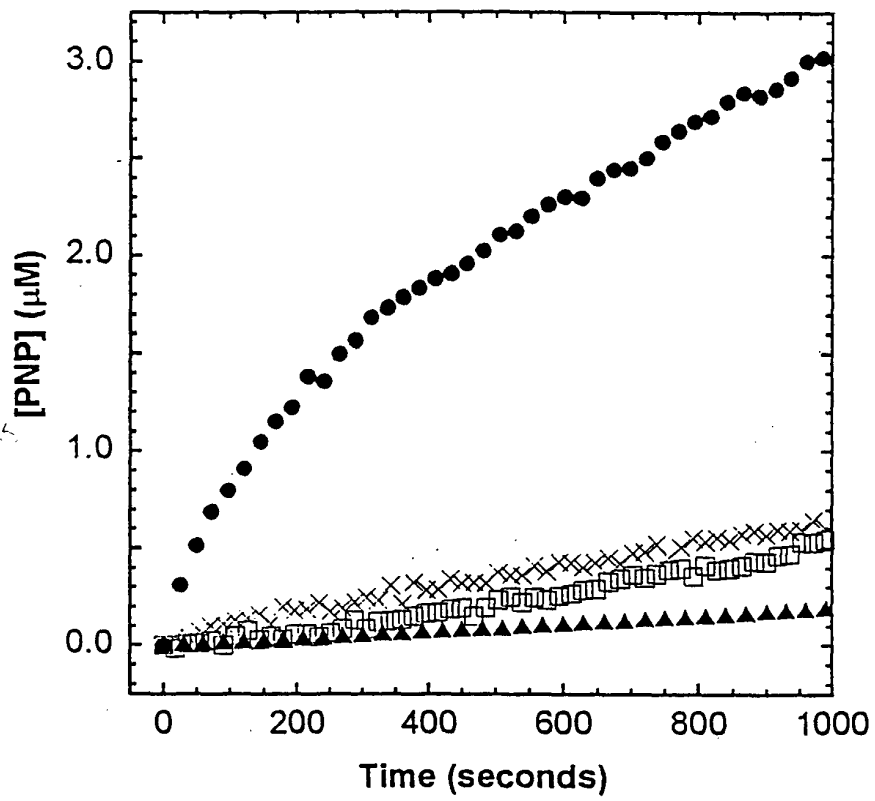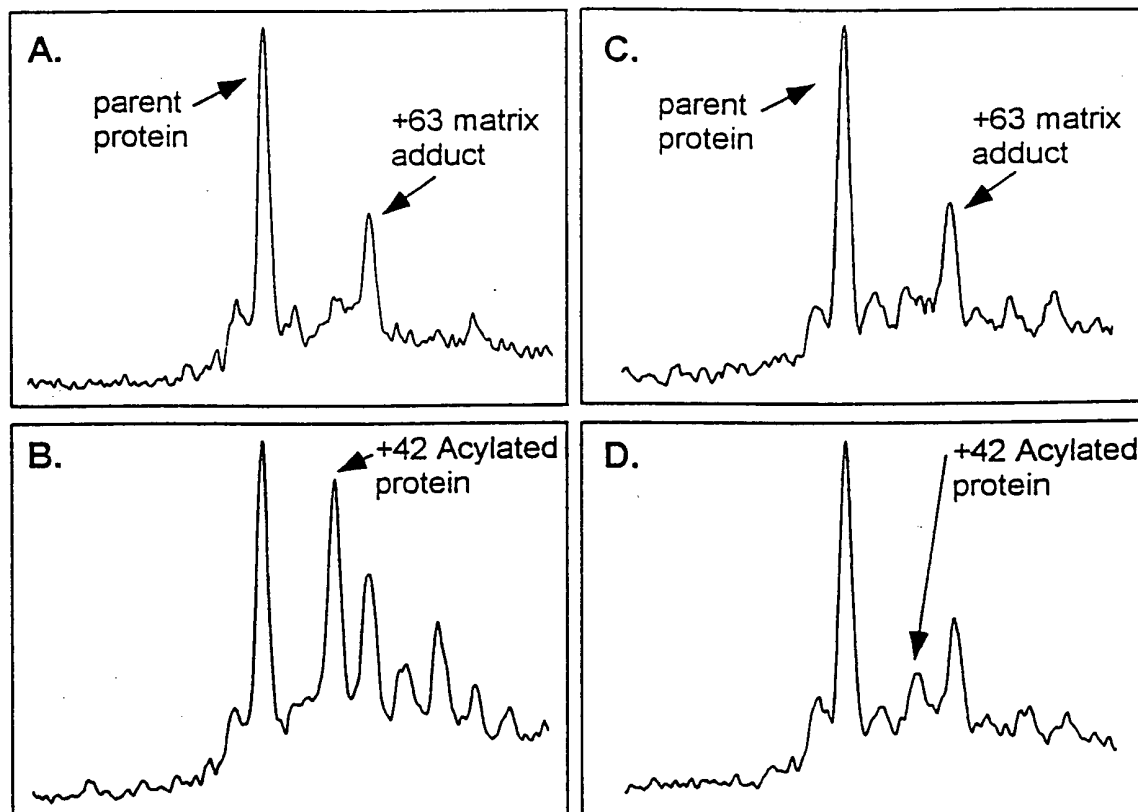A. parent protein
+63 matrix adduct

C. parent protein
+63 matrix adduct

B. +42 Acylated protein

D. +42 Acylated protein

Figure

9